Distribution of the resistance of nanowires with strong impurities

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Motivated by recent experiments on nanowires and carbon nanotubes, we study theoretically the effect of strong, point-like impurities on the linear electrical resistance R of finite length quantum wires. Charge transport is limited by Coulomb blockade and cotunneling. $\ln R$ is slowly self-averaging and non Gaussian. Its distribution is Gumbel with finite-size corrections which we compute. At low temperature, the distribution is similar to the variable range hopping (VRH) behaviour found long ago in doped semiconductors. We show that a result by Raikh and Ruzin does not apply. The finite-size corrections decay with the length L like $1/\ln L$. At higher temperatures, this regime is replaced by new laws and the shape of the finite-size corrections changes strongly: if the electrons interact weakly, the corrections vanish already for wires with a few tens impurities.

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Understanding the charge transport in materials with impurities has been a long standing problem which attracts new interest because of recent experiments on systems of nanoscopic size [1]. In the past, the case of doped semiconductors has been extensively studied [2]. Because of impurities, the electrons are, in equilibrium, in localized states. These states are randomly spread in energy and space. At low temperature, conduction results of a sequence of thermally activated hops of the charge carriers, which tunnel from one state to another, borrowing the energy difference from the phonons bath if needed. The spatial range of these hops results from a balance between tunneling (favoring short ranges) and activation (finding a state close to the Fermi level is more likely if the range is long). As a consequence, the low-field resistance R of amorphous semiconductors follow Mott's VRH law, $\ln R \sim T^{-1/(D+1)}$ in dimension D, with peculiarities in the special case of 1D [3, 4]. In presence of long-range Coulomb repulsion, as for crystalline semiconductors, the states close to the Fermi surface are rare and this law must be replaced at very low temperatures by the Shklovskii-Efros VRH law, $\ln R \sim T^{-1/2}$ [2].

Here we deal with 1D systems of nanoscopic cross-sections (nanowires) with point-like, strong impurities, and repulsive interactions between the electrons, at low applied electric field. In a pure nanowire, or between two impurities, the physics is described by the Tomonaga-Luttinger liquids (LL) model rather than a Fermi liquid because, in a 1D fermionic system, the excitations have a bosonic character. The case of a few strong impurities, or of a uniform density of weak impurities, have been studied [5, 6]. R was found to behave like powers of T at least in some regimes, with exponents which depend on the interaction parameter K of the LL. As was recently shown [7], in the case of many strong impurities, Coulomb blockade [1] and statistical effects yield different laws: at low temperature, a VRH-like regime is predicted, while at medium temperature a new, more complicated law (which can, on a small range of T, look like a power law) should replace it.

In this Letter, we first confirm numerically the existence of these two regimes for the average of $\ln R$. But they might be hard to distinguish due to huge sample to sample fluctuations. Therefore, we study the full distribution of $\ln R$. R and $\ln R$ are very slowly self-averaging and non Gaussian. Unless the wires are very long, the distribution of $\ln R$ is Gumbel with corrections that decay like $1/\ln L$ at low T. They are much weaker at medium T and have a different shape. We think this will help uncover experimentally the two regimes. Finally, we discuss the ergodicity hypothesis often used in experimental studies.

Our plan is the following: after introducing the model and the simulation technique, we show numerically that each sample has a high T regime where its resistance is proportional to the length and a "non extensive" regime where the voltage drop occurs essentially on a few *breaks*. We check the validity of a percolation-like approximation to R. Then we give our conclusions for the average of $\ln R$ and derive the distribution of $\ln R$.

Model. Our model is similar to the one of Refs. [8, 9]. We consider spinless electrons. Their interactions are short range because of screening by a nearby gate, which gives a finite capacitance per unit length C to the nanowires. Each wire is cut into a series of weakly coupled quantum dots by N impurities. They are placed randomly according to a Poisson process with mean spacing $\overline{l}$ large compared to the Fermi wavelength λ_F. In the quasiclassical limit, which is relevant because the impurities are strong, each dot j can only have an integer number, q_j, of electrons. Thus the charge transport proceeds by discrete hops, like in disordered semiconductors, and is limited by activation and tunneling. But unlike the localized states in the VRH model, here the energies of the states are correlated with their positions. Indeed, in the ground state, q_j is the closest integer $q_j^{(0)}$ to the mean charge $Q_j = l_j/\lambda_F + \mu/\Delta_j$, where μ is the chemical potential and $\Delta_j = 1/(Cl_j)$ is the charg-

ing energy (we use $e = k_B = 1$). The energy of dot j is $E_j(q_j) = (q_j - Q_j)^2 \Delta_j/2$ [6]. The typical charging energy $\Delta := 1/(\bar{l}C)$ is the natural energy scale of the problem. In addition, each charged excitation $q_j \neq q_j^{(0)}$ may itself be neutrally excited by an energy difference $\sim K\Delta_j$.

Having in mind experiments where a four-point measurement is performed [1], we do not pay attention to the contacts between the wire and the two leads. We assume for convenience that each impurity has the bare transparency $1/(e\pi) \approx 0.12$. According to [9, 11, 12], because of the LL effects, its *effective* tunneling transparency may be found by an instanton calculation, yielding $\exp(-s_{j,j+1})$ with $s_{j,j+1} = 1 + (K^{-1} - 1)(\sigma_{j-1} + \sigma_j)$ with $\sigma_j = \ln[K/(C\lambda_F)/\max(K\Delta_j, T)]$. The tunneling process is limited by neutral excitations at low T and by thermal fluctuations at high T. This extends readily to the probability $\exp(-s_{j,k})$ of the cotunneling of $k - j$ electrons, each through one of the impurities $j, \ldots, k-1$ (which is formally equivalent to the hop of one electron from the dot j to the dot k). At low temperatures, cotunneling allows to shortcut the narrow dots with high charging energy — this is why $\ln R$ increases slower than $1/T$ as T goes to 0.

Putting things together, we find the probability that an electron hops from dot j at x_j with initial charge q_j to dot k at x_k with initial charge q_k under field F:

$$w_{j,q_j,k,q_k} = e^{-s_{j,k}} \gamma_0 E \left[\exp(E/k_B T) - 1\right]^{-1} \qquad (1)$$

where $E = E_j(q_j - 1) - E_j(q_j) + E_k(q_k + 1) - E_k(q_k) - eF(x_k - x_j)$. The energy difference $E \gtrless 0$ is provided/absorbed by the phonons bath; the field F favors one hopping direction. γ_0 depends on the coupling with phonons [13].

In a steady regime, the average occupation probability of each state should be constant, therefore we write down for each state a balance equation between incoming and outgoing charge flows. Solving this in a general out-of-equilibrium setting is difficult, but, following the idea of Miller and Abrahams [13], we restrict to the small F regime and simplify these equations to the first order in F. The resulting equations are the Kirchhoff's laws for a resistor network between nodes labeled by j, q_j. In the following we are concerned with the low temperature regime $T \lesssim 10\Delta$ and we assume that only the first two charged excitations on each dot play a role. If this may not be true for all dots, it will certainly be the case for the dots which contribute the most to the resistance by their high charging energy. Moreover, we further simplify [7] to a network with one node per dot j and resistances $R_{j,k}$ equal to the minimum over q_j and q_k of the resistances between the states j, q_j and k, q_k. In this network, each node is connected to all others, although connections between remote dots are likely to be very resistive.

Simulations. We performed simulations by drawing at random the positions of the impurities of 10000 wires for each value of K, impurities number N and mean spacing $\bar{l}$. The low field resistance R of each wire is computed as the resistance of the equivalent network defined above; more precisely, we took care to manipulate $\ln R$ rather than R to prevent overflows at low T where R become huge; arbitrary precision arithmetics was used when needed to extract subdominant values. Simple linear solving of the Kirchhoff's equations fails at low temperatures because of numerical instabilities, but repeatedly eliminating one node of the network by applying a generalized star-triangle transformation [14] until only two nodes are left is efficient and stable.

For each wire, we also computed the resistance of the "best path", R_{bp}, which is the less resistive of the subnetworks without loops connecting the nodes 0 and $N+1$ and going always in the same direction, in analogy with the percolation approach to VRH [2]. A link in the best path is termed a *hop*. We found that $\ln R_{bp}$ is a very good approximation of $\ln R$ up to $T \sim 10\Delta$. Clearly, $R_{bp} > R$ because the full network has derivations around the best path. Empirically, $\ln R_{bp}/\ln R < 1.01$ always, and this ratio goes to 1 as T decreases. On our curves the averages of $\ln R_{bp}$ and $\ln R$ can't be distinguished. In the following we use R_{bp} for our analytical discussion because it is a *sum* of individual resistances.

From the simulations we conclude first that each sample has two well separated regimes: at high T the voltage drop is almost uniform and the resistance $R_{bp} \approx R$ is extensive (proportional to the length), but at low T the voltage drops mainly in one or a few regions, the *breaks* (Fig. 1), which makes R non extensive unless the wire is extremely long [15]. The positions of the breaks strongly depend on T and their width increases as T goes to zero and cotunneling through more and more impurities takes place. Fig. 1 shows this for one particular sample but it is true for all but pathological samples and for all values of K. The very low temperature regime $T \leq 0.01\Delta$ is cut into sample-specific ranges where $R(T)$ is activated, as was observed experimentally [1]: in each range of temperature, a different break fixes the voltage drop.

The second conclusion is a confirmation of the results of [7] for the average over many samples $\langle \ln R \rangle$: a VRH-like law $\langle \ln R \rangle \sim 1/\sqrt{T}$ holds at low T but has to be replaced by a new regime at intermediate T where $1/\langle \ln R \rangle$ is a affine in $\ln T$ (Fig. 2). However, unless the wire is very long, the temperature range where this new, non VRH-like law can be observed is small and it is in the cross-over between low and high temperatures (cotunneling and sequential tunneling), so that distinguishing the two laws is hard, all the more than the sample to sample fluctuations are large (Fig. 2). But we shall see that looking at the full distribution of $\ln R$ may help.

Analytical results for the distribution of $\ln R$. From now on, we restrict to the low T regime, where breaks are observed. Taking for simplicity uniform s and $\lambda_F = 0$, and neglecting correlations between hops, the probability

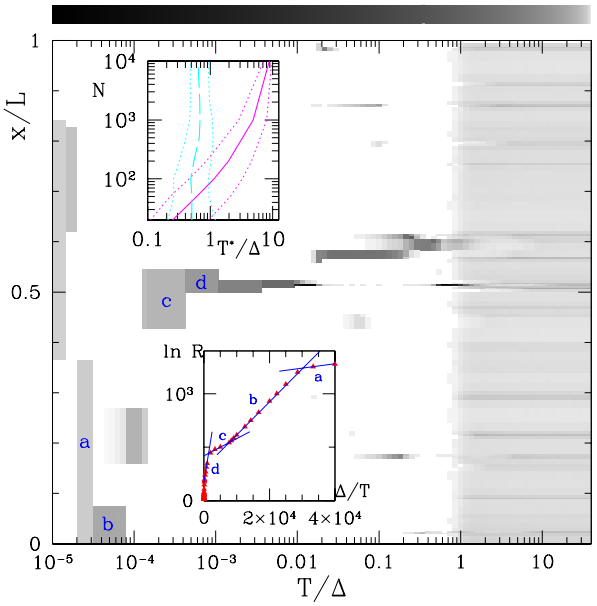

FIG. 1: The gradient of the electrical potential $V(x)$ along the best path in one random sample with $N = 100$ impurities, interaction parameter $K = 0.3$ and mean impurities spacing $\overline{l} = 10^3 \lambda_F$. For each value of the temperature T, we apply a voltage unity to the wire and we compute the gradient V' of V on each hop along the best path (see text). Then we color this hop with a grey intensity depending on V' (the bar above the figure indicates the intensity coding: white is null gradient and black is the maximal gradient over the whole figure). **Top inset:** The sum of the squares of the voltage drop of each hop along the best path is 1 at low temperature (one hops dominates) and $1/N$ at high temperature (N hops with drop $1/N$). For each of 10^4 samples from the same distribution, we look for the temperature T^* where it is equal to $1/\sqrt{N}$. This separates the non-extensive and extensive R regimes (see text). Strong lines: median value of T^* for several N values (solid: $K = 0.1$, dashed: $K = 0.7$). Dotted lines: boundaries of the 68% confidence interval on T^* at a given N. **Bottom inset:** Plot of $\ln R$ w.r.t. $1/T$. The curve is made of activated segments. In each one, the voltage drop occurs in one break which is identified by a letter on the main plot.

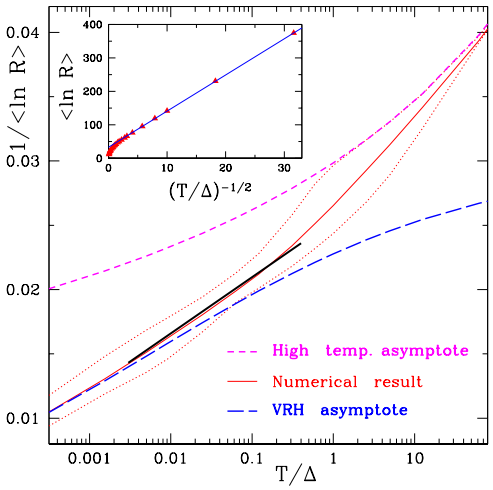

FIG. 2: Solid line: numerical results for the inverse of the average of $\ln R$ over 10^4 wires similar to the one of Fig. 1 as a function of T/Δ. The error bars are smaller than the line's thickness. The thin, dotted lines above and below indicate the boundaries of the 68% confidence interval at each temperature. Strong short-dashed line: high T asymptote and upper bond, reached when the electrons tunnel sequentially through all impurities. Strong long-dashed line: low T asymptote where $\ln(R)$ follows the VRH law, as found from the inset. The thick straight line indicates the validity of the new law predicted in [7] in some range of T. **Inset.** Dots: plot of the average $\ln R$ w.r.t. $\sqrt{\Delta/T}$ to show that, at low T, the VRH law is obeyed. The error bars are smaller than the symbols' size. Straight line: linear fit , which is used on the main plot as VRH asymptote.

that a given hop on the best path has $\ln R < u$ is

$$P\{R < e^u\} = 1 - \prod_{j=1}^{k} f[\frac{T}{\Delta}(\ln u - j\, s)] \text{ with } k = \lfloor u/s \rfloor \quad (2)$$

where [7] $f(x) := 1 - x\,[1 - \exp(-1/x)]$. The number n of hops in a sample is proportional to N (at low T, $n \approx \sqrt{sT/\Delta}N$) and, because of the equivalence of statistical ensembles, we can replace n or N by L in our asymptotic estimations. The most resistive hop has typically a resistance $R_{\max}$ such that $P\{R < R_{\max}\}^n \approx 1/2$. As long as $R_{\max}$ is large compared to the average hop resistance times n [16], we are in the non extensive R regime, $R_{bp} \approx R_{\max}$ — this regime extends at least to wires with several tens of thousands of impurities. If $R_{bp}/s \gtrsim 6$, $-\ln P[R > e^u]$ is well approximated by an integral, which itself takes two forms [7]: (a) $Tu^2/(s\Delta)$ if $uT/\Delta \ll 1$ and (b) $(u/s)\ln(uT/\Delta)$ if $uT/\Delta \gg 1$. The conditions $R_{bp}/s \gg 1$ and $T/\Delta \ln R_{bp} \ll 1$ are always fulfilled at (very) low temperatures, say $T \leq 0.001\Delta$. Furthermore, we verified numerically that the cumulative distribution function (CDF) of $\ln R$ of the hops along the best path of the wires (with nonuniform s) is in very good agreement with the shape $\exp(-u^2)$ once rescaled. Then $\ln R \approx \ln R_{bp}$ has for large n a Gumbel distribution because it is the maximum of n random variables with exponential decay of the probability density [17, 18]. Its average behaves like $\sqrt{s(\ln n)\Delta/T}$ and its standard deviation σ like $a/2/\sqrt{(\ln n)T/(\Delta s)}$ where $a := \pi/\sqrt{6}$, which is similar to the results of Lee *et al.* for the VRH model [4] and agrees with the low T result of [7]. Both R and $\ln R$ are non gaussian but self-averaging. We prefer to study $\ln R$ because it is easier to sample numerically. We computed the CDF of the centered and reduced $\ln R$ with finite n corrections [19]:

$$P\{\frac{\ln R - \langle \ln R \rangle}{\sigma} < x\} = \exp[-g(x)]\{1 - \quad (3)$$
$$g(x)[\pi^2/24(1-x^2) + x\zeta(3)/(2p)]/\ln n + \mathcal{O}[1/(\ln n)^2]\}$$

where $g(x) = \exp(-\gamma - a\,x)$, $\zeta(3) \approx 1.202$ and $\gamma \approx 0.577$.

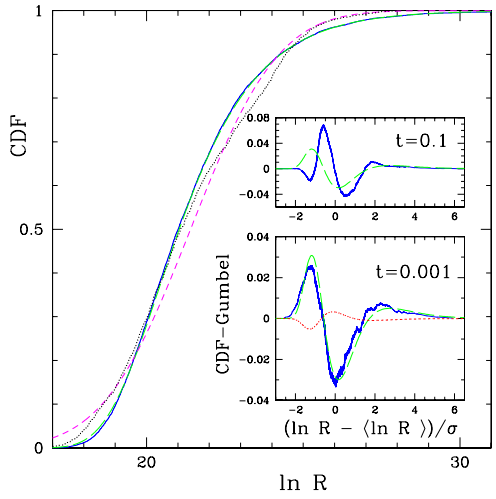

FIG. 3: Solid line: CDF of $\ln R$ for wires with $N = 100$ impurities, $K = 0.7$ and $\overline{l}/\lambda_F = 1000$ at temperature $T = 0.1\Delta$ from our simulation. Dotted line: the same for one sample but μ varying uniformly in the rage $-1..1$ to show that the ergodic hypothesis is only approximate. Long/short dashed line: Gumbel/Gauss distributions having the same average and variance than this CDF. The Gumbel distribution is almost superimposed on the data. **Insets.** Solid line: finite-size effects for the same wires but $K = 0.3$ and at $T = 0.1\Delta$ resp. 0.001Δ (difference between the CDF of the centered and reduced $\ln R$, and a Gumbel distribution). Long dashes: eq. (3) with $n = 100$. Dots: shape of the finite-size effects after Raikh and Ruzin's result.

This expression is successfully compared to the numerical CDF of $\ln R$ in the inset of Fig. 3. Since $1/\ln n$ goes slowly to zero, the actual $\ln R$ of each sample will likely lie away from the average $\langle \ln R \rangle$ even if n gets large. This is why activated segments are still visible on long wires.

Pursuing the work of Lee *et al.*, Raikh and Ruzin [15] evaluated the distribution of $\ln R$ in the case of 1D VRH. Interestingly, their result tends to a Gumbel law for very short wires or at very low T. But the finite-size effects are in $1/N^2$ and do not match eq. (3), nor our numerical results (bottom inset of Fig. 3).

At not so low temperatures, say $T > 0.01\Delta$, the CDF of individual hops doesn't agree with form (a) above but, if interactions are not too strong, with form (b). The VRH-like law $\langle \ln R \rangle \sim 1/\sqrt{T}$ is replaced by $\langle \ln R \rangle \approx s \ln n / \ln[(sT/\Delta)\ln n]$ where the number of hops n is proportional to L as before. The difference between the averages in the two regimes is small compared to the fluctuations $\sigma \sim 1/\ln\ln L$. But a strong change in the finite-size effects of the CDF of $\ln R$, which is Gumbel-like, should be easy to detect: their amplitude is reduced by $\ln[(sT/\Delta)\ln n]$ *i.e.* more than 3 in our data and their shape is changed. Fig. 3 shows that, for $K = 0.7$ and only $N = 100$ impurities one can't tell the difference between the CDF of $\ln R$ and a Gumbel CDF. For stronger interactions (smaller K), say $K = 0.3$, a typical break has only a few impurities, (b) is not valid, and the CDF is hard to characterize, but the deviations from a Gumbel law can't be confused with the formula (3) of the VRH case (top inset of Fig. 3) and might still be used as an evidence of strong impurities in a LL wire.

In an experimental study of the distribution of $\ln R$, it is common to measure R for the same sample but several values of the gate potential: this changes μ, and the activation energies strongly depend on μ. This was argued to yield the same results as using many samples (see [20] and references therein). However, in addition to varying μ, we recommend to use as many samples as possible because we found numerically that this ergodicity hypothesis is only approximate and may lead to systematic errors (Fig. 3).

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